

Compact Rational Krylov Methods for the Nonlinear Eigenvalue Problem

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Abstract

We present a new framework of Compact Rational Krylov (CORK) methods for solving the nonlinear eigenvalue problem (NLEP):

$$A(\lambda)x = 0,$$

where $\lambda \in \Omega \subseteq \mathbb{C}$ is called an eigenvalue, $x \in \mathbb{C}^n \setminus \{0\}$ the corresponding eigenvector, and $A : \Omega \rightarrow \mathbb{C}^{n \times n}$ is analytic on Ω . Linearizations are used for many years for solving polynomial eigenvalue problems [5]. The matrix polynomial $P(\lambda) = \sum_{i=0}^d \lambda^i P_i$, with $P_i \in \mathbb{C}^{n \times n}$, is transformed to a linear pencil $L(\lambda) = X - \lambda Y$, with $X, Y \in \mathbb{C}^{dn \times dn}$, so that there is a one-to-one correspondence between the eigenvalues of $P(\lambda)x = 0$ and $L(\lambda)u = 0$.

For the general nonlinear case, i.e., nonpolynomial eigenvalue problem, $A(\lambda)$ is first approximated by a matrix polynomial [1, 4, 7] or rational matrix polynomial [2] and then a convenient linearization is used. The linearizations used in the literature can all be written in the following form

$$L(\lambda) = \mathbf{A} - \lambda \mathbf{B},$$

where

$$\mathbf{A} = \begin{bmatrix} A_0 & A_1 & \cdots & A_{d-1} \\ M \otimes I_{n \times n} \end{bmatrix}, \quad \mathbf{B} = \begin{bmatrix} B_0 & B_1 & \cdots & B_{d-1} \\ N \otimes I_{n \times n} \end{bmatrix},$$

with $\mathbf{A}, \mathbf{B} \in \mathbb{C}^{dn \times dn}$, $A_i, B_i \in \mathbb{C}^{n \times n}$, and $M, N \in \mathbb{C}^{(d-1) \times d}$. Note that the pencil (\mathbf{A}, \mathbf{B}) also covers the dynamically growing linearization pencils used in [3, 4, 7, 2]. The construction of the (rational) polynomial approximation of $A(\lambda)$ can be obtained using results on approximation theory or can be constructed dynamically during the solution process. The last two years, we developed various variants of the rational Krylov method based on these ideas [7, 2].

The major disadvantage of methods based on linearizations is the growing memory cost with the iteration count. It is possible to reduce this cost in specific cases, but in general, the memory cost is proportional to the degree of the polynomial. However, we can exploit the kronecker structure of the part below the first block row of the pencil (\mathbf{A}, \mathbf{B}) such that the memory cost is not proportional with the degree of the polynomial any more and only grows linearly with the iteration number. We therefore present the CORK family of rational Krylov methods, which use a generalization of the compact Arnoldi decomposition, proposed in [6]. All these methods construct a subspace $\mathbf{V} \in \mathbb{C}^{dn \times k}$, represented by two smaller matrices $Q \in \mathbb{C}^{n \times r}$ and $\mathbf{U} \in \mathbb{C}^{dr \times k}$ with orthonormal columns and $r \leq d + k$, such that

$$\mathbf{V} = (I_{d \times d} \otimes Q)\mathbf{U}.$$

In this way, the extra memory cost due to the linearization of the original eigenvalue problems is negligible.

For large-scale NLEPs, we present a two-level approach: at the first level, the large-scale NLEP is projected yielding a small (nonlinear) eigenvalue problem at the second level. Therefore, the method consists of two nested iterations. In the outer iteration, we construct an orthogonal basis Q and project $A(\lambda)$ or $L(\lambda)$ onto it. In the inner iteration, we solve the projected small linear eigenvalue problem

$$\hat{L}(\lambda)u = 0, \quad \hat{L}(\lambda) = (I_{d \times d} \otimes Q)^* L(\lambda) (I_{d \times d} \otimes Q),$$

or the projected small NLEP

$$\hat{A}(\lambda)x = 0, \quad \hat{A}(\lambda) = Q^*A(\lambda)Q.$$

The partial Schur decomposition of the linearization allows for efficient and reliable locking, purging and restarting. We translate these operations on the (approximate) invariant pairs of the underlying nonlinear eigenvalue problem, which leads to a two-level approach. We also illustrate the methods with numerical examples and give a number of scenarios where the methods performs very well.

References

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